Final Scientific Report

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BARD Project Number: IS-4090-08

Date of Submission of the report: December 2nd, 2012

Project Title: Development of Predictive Tools for Contaminant Transport through Variably Saturated Heterogeneous Composite Porous Formations

Investigators	Institutions
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Keywords
Uncertainty analysis, numerical simulation, stochastic analysis, unsaturated zone

Abbreviations
CDF - cumulative density function, CTES - coarse-textured embedded soil, FTES - fine-textured embedded soil, MCS - Monte Carlo simulation, PDF - probability density function.

Budget: IS: $ 132,000 US: $ 172,000 Total: $ 194,000

Signature
Principal Investigator

Signature
Authorizing Official, Principal Institution

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Publication Summary (numbers)

	Joint IS/US authorship	US Authors only	Israeli Authors Only	Total
Refereed (published, in press, accepted) BARD support acknowledged		5	4	9
Submitted, in review, in preparation		3 (p)	1 (r)	4
Invited review papers				
Book chapters				
Books				
Master theses				
Ph.D. theses		2		
Abstracts				
Not refereed (proceedings, reports, etc.)				

Postdoctoral Training: List the names and social security/identity numbers of all postdocs who received more than 50% of their funding by the grant.

Cooperation Summary (numbers)

	From US to Israel	From Israel to US	Together, elsewhere	Total
Short Visits & Meetings	1			1
Longer Visits (Sabbaticals)				

Description of Cooperation:
The US and the Israeli research groups conducted their research from a common design scheme that produced different perspectives on common problems. Water flow and solute transport on the field scale are of sufficient complexity, so that current methods are often found lacking in representing these processes under natural conditions. Our research was designed to create new theoretical and practical tools for addressing the problems created by the spatial variability, and, concurrently, uncertainty in the soil hydraulic properties. Wherever possible, the US and the Israeli investigators used complementary approaches to the same problem to maximize the effectiveness of the investigation. Information exchange between the teams during the research project was performed routinely via electronic mail communication. The American collaborating investigator traveled to Israel towards the end of the project in order to discuss the project results and outlines for the final report

Patent Summary (numbers)

	Israeli inventor only	US inventor only	Joint IS/US inventors	Total
Submitted				
Issued				
Licensed				

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Abstract

The vadose (unsaturated) zone forms a major hydrologic link between the ground surface and underlying aquifers. To understand properly its role in protecting groundwater from near surface sources of contamination, one must be able to analyze quantitatively water flow and contaminant transport in variably saturated subsurface environments that are highly heterogeneous, often consisting of multiple geologic units and/or high and/or low permeability inclusions.

The specific objectives of this research were: (i) to develop efficient and accurate tools for probabilistic delineation of dominant geologic features comprising the vadose zone; (ii) to develop a complementary set of data analysis tools for discerning the fractal properties of hydraulic and transport parameters of highly heterogeneous vadose zone; (iii) to develop and test the associated computational methods for probabilistic analysis of flow and transport in highly heterogeneous subsurface environments; and (iv) to apply the computational framework to design an "optimal" observation network for monitoring and forecasting the fate and migration of contaminant plumes originating from agricultural activities.

During the course of the project, we modified the third objective to include additional computational method, based on the notion that the heterogeneous formation can be considered as a mixture of populations of differing spatial structures.

Regarding uncertainly analysis, going beyond approaches based on mean and variance of system states, we succeeded to develop probability density function (PDF) solutions enabling one to evaluate probabilities of rare events, required for probabilistic risk assessment. In addition, we developed reduced complexity models for the probabilistic forecasting of infiltration rates in heterogeneous soils during surface runoff and/or flooding events

Regarding flow and transport in variably saturated, spatially heterogeneous formations associated with fine- and coarse-textured embedded soils (FTES- and CTES-formations, respectively).We succeeded to develop first-order and numerical frameworks for flow and transport in three-dimensional (3-D), variably saturated, bimodal, heterogeneous formations, with single and dual porosity, respectively.

Regarding the sampling problem defined as, how many sampling points are needed, and where to locate them spatially in the horizontal x_2x_3 plane of the field. Based on our computational framework, we succeeded to develop and demonstrate a methdology that might improve considerably our ability to describe quntitaively the response of complicated 3-D flow systems.

The results of the project are of theoretical and practical importance; they provided a rigorous framework to modeling water flow and solute transport in a realistic, highly heterogeneous, composite flow system with uncertain properties under-specified by data. Specifically, they: (i) enhanced fundamental understanding of the basic mechanisms of field-scale flow and transport in near-surface geological formations under realistic flow scenarios, (ii) provided a means to assess the ability of existing flow and transport models to handle realistic flow conditions, and (iii) provided a means to assess quantitatively the threats posed to groundwater by contamination from agricultural sources.

Achievements

Significance of Main Scientific Achievements or Innovations

We were able to meet all of our goals in this BARD project, as articulated in the project proposal objectives, except objective (iv). In this section, we discuss the significance of our results relative to the original expectations. Considering the quantification of water flow and contaminant transport in variably saturated subsurface environments that are highly heterogeneous, the US investigators spent a considerable effort developing and testing novel methods for uncertainly analyses:

1 The US team [*Wang et al*., 2009] conducted a series of flow and transport simulations, in which daily data from a weather station serve as input, to demonstrate that precipitation patterns typical of (semi-)arid regions make the reliance on annual data questionable. It was demonstrated that the accuracy of temporally averaged predictions is influenced by the degree of nonlinearity of the Richards equation describing flow in partially saturated porous media. Additional errors are introduced when one ignores topographical and/or urban features that tend to focus and increase local infiltration rates.

2. The US team [*Wang and Tartakovsky*, 2011a,b] analyzed two reduced complexity models of infiltration into heterogeneous soils with uncertain hydraulic properties. For both models, semi-analytical solution of the infiltration-rate PDF was derived. This approach goes beyond standard approaches, which typically just compute the first two ensemble moments of the system states (*e.g*., pressure, saturation, and flux), and enables one to evaluate probabilities of rare events (distribution tails) for probabilistic risk assessment. The relative effects of different sources of uncertainty and the degree of cross-correlation between various soil parameters on the infiltration-rate PDFs were investigated. Monte Carlo simulations (MCS) of the Richards equation were performed at the end to serve as a benchmark for comparison with the PDFs obtained from the two reduced complexity models.

3. The US team [*Wang and Tartakovsky*, 2012] developed a probabilistic approach to quantify parametric uncertainty in models of overland flow. The approach relies on the derivation of a deterministic equation for the cumulative density function (CDF) of a system state, in which probabilistic descriptions (probability density functions or PDFs) of system parameters and/or initial and boundary conditions serve as inputs. In

contrast to PDF equations, which are often used in other contexts, CDF equations allow for straightforward and unambiguous determination of boundary conditions with respect to sample variables. The accuracy and robustness of solutions of the CDF equation for one such system, the Saint-Venant equations, were investigated via comparison with Monte Carlo simulations.

4. The US team [*Barajas-Solano and Tartakovsky*, 2013] developed an accurate and numerically efficient approach to compute Green's functions for transport processes in heterogeneous composite media. Focusing on steady Richards' equation with uncertain discontinuous coefficients, the approach relied on a regularization technique to obtain an associated regular problem, which can be solved using standard finite element methods. Numerical experiments were performed to assess the performance of the regularization approach and to evaluate the effects of strong coefficient discontinuities on the Green's function behavior.

The Israeli research team concentrates on: (i) developing and testing novel methods for analyzing flow and transport in variably saturated, heterogeneous, unimodal and bimodal, composite formations, and, (ii) testing of a theoretical framework for the solute sampling design problem**,** developed by the Israeli team, considering transport of nitrate, chloride and a tracer solute in a three-dimensional (3-D), spatially heterogeneous, variably saturated soil, originating from a citrus orchard irrigated with treated sewage water (TSW):

1. The Israeli team [*Russo*, 2009] employed first-order analysis in order to analyze the PDF of the saturation-dependent, log-conductivity, logK, in variably saturated, composite, bimodal, heterogeneous formations. The resultant logK PDF depends on mean pressure head, H, in a manner which depends on the texture of the embedded soil relative to that of the background soil. It was demonstrated that in CTES-formations, diminishing water saturation may lead to a highly skewed logK PDF, which, in turn, may exhibit an exceedingly large tail associated with the small K values.

2. The Israeli team [*Russo*, 2010] employed first-order, Lagrangian-stochastic framework of vadoze zone transport, in order to further invesigate solute spread and breakthrough in a 3-D, variably saturated, composite, bimodal, heterogeneous, formations.Results of our first-order analyses (confirmed by a series of detailed

numerical simulations of the flow and transport in three-dimensional, heterogeneous, bimodal, variably saturated formations),demonstrated that in steady-state flow conditions, under relatively wet and dry conditions, FTES- and CTES-formations, respectively, may induce preferential flow, and, consequently, highly skewed solute BTC. The effect of the embedded soil's texture, however, diminished substantially at intermediate water saturations, relevant to realistic transient flow conditions associated with substantial redistribution periods and water uptake by plant roots.

3. The Israeli team [*Russo*, 2012] employed a series of detailed numerical simulations of flow and transport in 3-D, variably saturated, composite, bimodal, heterogeneous formations in which part of the water-filled pore space is stagnant, in order to anlayze the effect of the interaction between the mobile and the immobile regions on solute transport. Results of the analyses suggest that mass exchange between the two regions masks features of the transport that exist in bimodal, one-region flow domains, related to characteristics of the unsaturated hydraulic conductivity in variably saturated bimodal, heterogeneous formations

4. The Israeli team [*Russo*, 2011], analyzed the effect of both the soil type and the pulse application date on solute movement and spreading in a 3-D, spatially heterogeneous, combined flow system subject to time-dependent, external forcing conditions, F(t), (characterized by a time period, τ_p), imposed the soil surface, and water uptake by plant roots, through a series of detailed, 3-D numerical simulations. Results of the analyses suggest that characteristics of the transport (i.e., solute displacement and spreading, first- and peak-arrival times) are soil- and pulse release date-dependent. The soil-dependent solute travel time PDF at a CP located in the vicinity of the water table, however, may be considered as essentially independent of the pulse release date, particularly in the fine-textured soil associated with mean travel time, τ_0 that substantially exceeds τ_p. Furthermore, for $\tau_0 > \tau_p$, the equivalent steady-state definition of the flow problem may be quite effective in describing the solute travel time PDF of the actual transport process occurring under non-monotonous, transient flow conditions.

5. The Israeli team [*Russo et al.*, 2012], analyzed water flow and transport of nitrate, chloride and a tracer solute in a 3-D, spatially heterogeneous, variably saturated soil, originating from a citrus orchard irrigated with treated sewage water (TSW) considering realistic features of the soil-water-plant-atmosphere system, through a series

of detailed, 3-D numerical simulations. Results of the 3-D simulations were used to assess their counterparts based on a simplified, deterministic1-D vertical simulation and on limited soil monitoring. Results of the analyses suggest that the information which may be gained from a single sampling point (located close to the area active in water uptake by the trees' roots), or from the results of the 1-D simulation, is insufficient for a quantitative description of the response of the complicated, 3-D flow system. Both may considerably underestimate the movement and spreading of a pulse of a tracer solute, and might considerably underestimate the groundwater contamination hazard posed by nitrate, and, particularly, by chloride moving through the vadose zone. It was shown, however, that an additional sampling point, located outside the area active in water uptake, may substntailly improve the quantitative description of the response of the complicated 3-D flow system.

Two of the major achievements of this project are that we succeeded to: (i) develop probability density function solutions enabling one to evaluate probabilities of rare events, required for probabilistic risk assessment; and (ii) develop reduced complexity models for the probabilistic forecasting of infiltration rates in heterogeneous soils during surface runoff and/or flooding events. In addition, our findings regarding (i) the combined effect of the embedded soil's texture and water saturation on solute spread and breakthrough in variably saturated, heterogeneous composite formations; and (ii) the quantification of chloride and nitrate transport in the vadose zone, beneath orchards irrigated with TSW, are novel and have practical implications regarding groundwater contamination.

Details of cooperation

The US and the Israeli research groups conducted their research from a common design scheme that produced different perspectives on common problems. Water flow and solute transport on the field scale are of sufficient complexity, so that current methods are often found lacking in representing these processes under natural conditions. Our research was designed to create new theoretical and practical tools for addressing the problems created by the spatial variability, and, concurrently, uncertainty in the soil hydraulic properties. Wherever possible, the US and the Israeli investigators used complementary approaches to the same problem to maximize the effectiveness of the investigation. Information exchange between the teams during the research project was

performed routinely via electronic mail communication. The American collaborating investigator traveled to Israel towards the end of the project in order to discuss the project results and outlines for the final report.

Appendix

1. Published papers

1. Barajas-Solano, D. A., and D. M. Tartakovsky, Computing Green's functions for flow in heterogeneous composite media, *Int. J. Uncert. Quant.*, 3(1), 39-46, 2013.

2. Russo, D**.,** On probability distribution of hydraulic conductivity in variably saturated bimodal heterogeneous formations. *Vadose Zone Journal* 8, 611-622, doi:10.2136/ vzj2008.011, 2009.

3. Russo, D**.,** First-order and numerical analyses of flow and transport in heterogeneous bimodal variably saturated formations. *Water Resour. Res*., 46, W06509, doi:10.1029/2009WR008307, 2010.

4. Russo, D**.,** The effect of pulse release date and soil characteristics on solute transport in a combined vadose zone-groundwater flow system: Insights from numerical simulations**.** *Water Resour. Res.* 47, W05532, doi:10.1029/2010WR010094, 2011.

5. Russo, D**.**, Numerical Analysis of Solute Transport in Variably Saturated Bimodal Heterogeneous Formations with Mobile-Immobile Porosity. *Adv. Water Resour.*, http://dx.doi.org/10.1016/j.advwatres.2012.05.017, 2012.

6. Wang, P., P. Quinlan and D. M. Tartakovsky, Effects of spatio-temporal variability of precipitation on contaminant migration in vadose zone, *Geophys. Res. Lett.*, 36, doi:10.1029/2009GL038347, L12404, 2009.

7. Wang, P. and D. M. Tartakovsky, Probabilistic predictions of infiltration into heterogeneous media with uncertain hydraulic parameters, *Int. J. Uncert. Quant.*, 1(1), 35-47, 2011.

8. Wang, P. and D. M. Tartakovsky, Reduced complexity models for probabilistic forecasting of infiltration rates, *Adv. Water Resour.*, 34, 375-382, 2011.

9. Wang, P., and D. M. Tartakovsky, Uncertainty quantification in kinematic-wave models, *J. Comp. Phys.*, 231(23), 7868-7880, 2012.

2. Submitted Papers

1. Russo, D. , A. Laufer, R. H. Shapira and D. Kurtzman, Assessment of Solute Fluxes Beneath an Orchard Irrigated with Treated Sewage Water: A numerical Study, *Water Resour. Res*. (under review), 2012.